THE WEAKLY-BOUND COMPLEX CH_4-H_2: OBSERVATION AND ANALYSIS OF INFRARED SPECTRA IN THE 350 AND 1311 cm^{-1} REGIONS

A.R.W. McKELLAR, *Steacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada*; D.A. ROTH, I. PAK, and G. WINNEWISSER, *I. Physikalisches Institut, Universität zu Köln, Zulpicherstrasse 77, 50937 Köln, Germany*.

Infrared spectra of the weakly-bound van der Waals complex CH_4-*para*H_2 have been observed and analyzed for the first time. Measurements were made using a long path (160-180 m) low temperature (61-92 K) absorption cell which was probed with a Bomem Fourier transform spectrometer (350 and 1311 cm^{-1}) or a tunable diode laser (1311 cm^{-1}). The partly resolved spectrum accompanying the $S_0(0)$ pure rotational transition of H_2 around 350 cm^{-1} was analyzed in terms of an approximate model to obtain the rotational and centrifugal distortion constants of the complex in its ground state. The high resolution spectrum accompanying the $R(0)$ transition of the ν_4 fundamental band of CH_4 near 1311 cm^{-1} was assigned in detail and analyzed using the Coriolis model used previously for analogous spectra of methane - rare gas complexes.[a] The effective intermolecular separation and dissocation energy of the complex in its ground state were determined to be about 4.12 Å and 28 cm^{-1}, respectively. Absorption due to CH_4-*para*H_2 has also been observed in the 1317 cm^{-1} region near the $R(1)$ transition of CH_4, but this is not yet analyzed.

[a] I. Pak, D.A. Roth, M. Hepp, G. Winnewisser, D. Scouteris, B.J. Howard, and K.M.T. Yamada, Z. Naturforsch. **53a**, 725 (1998).